3.2.3.2.7. *Halving subgroups and dichromatic (black-and-white) groups*

Any subgroup H of a group G of index 2, called a *halving subgroup*, is a normal subgroup. The decomposition of G into left cosets of H consists of two left cosets,

$$G = H \cup gH. \tag{3.2.3.33}$$

Sometimes it is convenient to distinguish elements of the coset gH from elements of the halving subgroup H. This can be achieved by attaching a sign (usually written as a superscript) to all elements of the coset. We shall use for this purpose the sign $^{\spadesuit}$. To aid understanding, we shall also mark for a while the elements of the group H with another sign, $^{\heartsuit}$. The multiplication law for these 'decorated elements' can be written in the following form:

$$g_1^{\heartsuit} g_2^{\heartsuit} = g_3^{\heartsuit}, \quad g_4^{\heartsuit} g_5^{\spadesuit} = g_6^{\spadesuit}, \quad g_7^{\spadesuit} g_8^{\heartsuit} = g_9^{\spadesuit}, \quad g_{10}^{\spadesuit} g_{11}^{\spadesuit} = g_{12}^{\heartsuit}. \tag{3.2.3.34}$$

Now we replace the label $^{\heartsuit}$ by a dummy 'no mark' sign (*i.e.* we remove $^{\heartsuit}$), but we still keep in mind the multiplication rules (3.2.3.34). Then the decomposition (3.2.3.33) becomes

$$G = H \cup g^{\spadesuit} H, \tag{3.2.3.33a}$$

since the coset $g^{\spadesuit}H$ assembles all marked elements and H consists of all bare elements of the group G.

The sign $^{\spadesuit}$ can carry useful additional information, *e.g.* the application of labelled operations $g^{\spadesuit}$ is connected with some changes or new effects, whereas the application of a bare operation brings about no such changes or effects.

The label $^{\spadesuit}$ can be replaced by various signs which can have different meanings. Thus in Chapter 3.3 a prime $'$ signifies a nontrivial twinning operation, in Chapter 1.5 it is associated with time inversion in magnetic structures, and in black-and-white patterns or structures a prime denotes an operation which exchanges black and white 'colours' (the qualifier 'black-and-white' concerns group operations, but not the black-and-white pattern itself). In Chapter 3.4, a star * denotes a transposing operation which exchanges two domain states, while underlining signifies an operation exchanging two sides of an interface and underlined operations with a star signify twinning operations of a domain twin. Various interpretations of the label attached to the symbol of an operation have given rise to several designations of groups with partition (3.2.3.34): *black-and-white*, *dichromatic*, *magnetic*, *anti-symmetry*, *Shubnikov* or *Heech–Shubnikov* and other *groups*. For more details see Opechowski (1986).

3.2.3.2.8. *Double cosets*

Let F_1 and H_1 be two proper subgroups of the group G. The set of all distinct products hg_jf, where g_j is a fixed element of the group G and f and h run over all elements of the subgroups F_1 and H_1, respectively, is called a *double coset of F_1 and H_1 in G*. The symbol of this double coset is $H_1g_jF_1$,

$$F_1 g_j H_1 = \{fg_jh \mid \forall f \in F_1, \forall h \in H_1\}, \quad g_j \in G,\ F_1 \subset G,\ H_1 \subset G, \tag{3.2.3.35}$$

where the sign $\forall$ means 'for all'.

In the symmetry analysis of domain structures, only double cosets with $H_1 = F_1$ are used. We shall, therefore, formulate subsequent definitions and statements only for this special type of double coset.

The fixed element g_j is called the *representative of the double coset $F_1g_jF_1$*. Any element of a double coset can be chosen as its representative.

Two double cosets are either identical or disjoint.

Proposition 3.2.3.6. The union of all distinct double cosets constitutes a partition of G and is called the *decomposition of the group G into double cosets of F_1*, since $F_1F_1 = F_1$. If the set of double cosets of F_1 in G is finite, then the decomposition of G into the double cosets of F_1 can be written as

$$G = F_1g_1F_1 \cup F_1g_2F_1 \cup \ldots \cup F_1g_qF_1. \tag{3.2.3.36}$$

For the representative g_1 of the first double coset $F_1g_jF_1$ the unit element e is usually chosen, $g_1 = e$. Then the first double coset is identical with the subgroup F_1.

A double coset $F_1g_jF_1$ consists of left cosets of the form fg_jF_1, where $f \in F_1$. The number r of left cosets of F_1 in the double coset $F_1g_jF_1$ is (Hall, 1959)

$$r = [F_1 : F_{1j}], \tag{3.2.3.37}$$

where

$$F_{1j} = F_1 \cap g_jF_1g_j^{-1}. \tag{3.2.3.38}$$

The following definitions and statements are used in Chapter 3.4 for the double cosets $F_1g_jF_1$ [for derivations and more details, see Janovec (1972)].

The inverse $(F_1g_jF_1)^{-1}$ of a double coset $F_1g_jF_1$ is a double coset $F_1g_j^{-1}F_1$, which is either identical or disjoint with the double coset $F_1g_jF_1$. The double coset that is its own inverse is called an *invertible* (*self-inverse*, *ambivalent*) *double coset*. The double coset that is disjoint with its inverse is called a *non-invertible* (*polar*) *double coset* and the double cosets $F_1g_jF_1$ and $(F_1g_jF_1)^{-1} = F_1g_j^{-1}F_1$ are called *complementary polar double cosets*.

The inverse left coset $(g_jF_1)^{-1}$ contains representatives of all left cosets of the double coset $F_1g_j^{-1}F_1$. If a left coset g_jF_1 belongs to an invertible double coset, then $(g_jF_1)^{-1}$ contains representatives of left cosets constituting the double coset $F_1g_jF_1$. If a left coset g_jF_1 belongs to a non-invertible double coset, then $(g_jF_1)^{-1}$ contains representatives of left cosets constituting the complementary double coset $(F_1g_jF_1)^{-1}$.

A double coset consisting of only one left coset,

$$F_1g_jF_1 = g_jF_1, \tag{3.2.3.39}$$

is called a simple *double coset*. A double coset $F_1g_jF_1$ is *simple* if and only if the inverse $(g_jF_1)^{-1}$ of the left coset g_jF_1 is again a left coset. For an invertible simple double coset $g_jF_1 = (g_jF_1)^{-1}$.

The union of all simple double cosets $F_1g_jF_1 = g_jF_1$ in the double coset decomposition of G (3.2.3.36) constitutes the normalizer $N_G(F_1)$ (Speiser, 1927).

A double coset that comprises more than one left coset will be called a *multiple double coset*. Four types of double cosets *FgF* are displayed in Table 3.2.3.1. The double coset decompositions of all crystallographic point groups are available in the software *GI★KoBo*-1 under *Subgroups\View\Twinning Group*.

Double cosets and the decomposition (3.2.3.36) of a group in double cosets are mathematical tools for partitioning a set of pairs of objects into equivalent classes (see Section 3.2.3.3.6). Such a division enables one to find possible twin laws and different types of domain walls that can appear in a domain structure resulting from a phase transition with a given symmetry descent (see Chapters 3.3 and 3.4).

More detailed introductions to group theory can be found in Budden (1972), Janssen (1973), Ledermann (1973), Rosen (1995), Shubnikov & Koptsik (1974), Vainshtein (1994) and Vainshtein *et*

Table 3.2.3.1. *Four types of double cosets*

	$FgF = gF$	$FgF \neq gF$
$FgF = (FgF)^{-1}$	Invertible simple	Invertible multiple
$FgF \cap (FgF)^{-1} = \emptyset$	Non-invertible simple	Non-invertible multiple

al. (1995). More advanced books on group theory are, for example, Bradley & Cracknell (1972), Hall (1959), Lang (1965), Opechowski (1986), Robinson (1982) and Speiser (1927). Parts of group theory relevant to phase transitions and tensor properties are treated in the manual of the software *GI★KoBo*-1. Representations of the crystallographic groups are presented in Chapter 1.2 of this volume and in the software *GI★KoBo*-1 (see the manual).

3.2.3.3. *Action of a group on a set*

3.2.3.3.1. *Group action*

A direct application of the set and group theory to our studies would hardly justify their presentation in the last two sections. However, an appropriate combination of these theories, called group action, forms a very useful tool for examining crystalline materials and domain structures in particular. In this section, the main concepts (action of a group on a set [a], orbits [o], stabilizers [s]) are explained and their application is illustrated with examples from crystallography, where the group G is either a crystallographic point group or space group (denoted $\mathcal{G}$, if necessary), and the set is the three-dimensional point space $E(3)$ [P], a crystal [C], a property tensor [T] and a subgroup of G [S]. Letters in square brackets in front of the sequential number of examples and definitions should aid navigation in the text.

Example [aP] 3.2.3.7. Crystals are objects in a three-dimensional space called point space. Points of this space form an infinite set which we denote $E(3)$. If one chooses a point O as the origin, then to each point $X \in E(3)$ one can assign the position vector $OX = \mathbf{r}$ of a vector space $V(3)$ [see, for example, *IT* A (2002), Part 8]. There is a one-to-one correspondence between points of the point space and corresponding position vectors of the vector space,

$$X \leftrightarrow OX = \mathbf{r}. \tag{3.2.3.40}$$

If one further selects three non-coplanar basic vectors $\mathbf{e_1}, \mathbf{e_2}, \mathbf{e_3}$, then the position vector $\mathbf{r}$ can be written as

$$\mathbf{r} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + x_3\mathbf{e}_3, \tag{3.2.3.41}$$

where x_1, x_2, x_3 are coordinates of the point X.

Let G be a point group. An operation (isometry) $g \in G$ transforms (moves) the point X to a point X' with the position vector

$$\mathbf{r}' = x'_1\mathbf{e}_1 + x'_2\mathbf{e}_2 + x'_3\mathbf{e}_3. \tag{3.2.3.42}$$

Coordinates of this image point are related to coordinates of the initial point by a linear relation,

$$x'_i = \sum_{j=1}^{3} D(g)_{ij}x_j, \quad i = 1, 2, 3, \tag{3.2.3.43}$$

where $D(g)_{ij}$ are components of a 3×3 matrix representing the operation g.

The described motion of the point X under the operation g can be formally expressed as a simple relation

$$gX = X', \quad g \in G, \quad X, X' \in E(3), \tag{3.2.3.44}$$

the exact meaning of which can be formulated in terms introduced in Section 3.2.3.1 as a mapping φ that assigns to an ordered pair (g, X) a point X' of the set $E(3)$,

$$\varphi : (g, X) \mapsto X', \quad g \in G \text{ and } X, X' \in \mathsf{A}. \tag{3.2.3.45}$$

The mapping φ – *i.e.* a prescription for how to determine from g and X the resulting point X' – is defined by (3.2.3.40) to (3.2.3.43). The relation (3.2.3.44) should be considered as only a shorthand version of the explicit relation (3.2.3.45).

The action of a group on a set generalizes the described procedure to any group and any set. In this section, we shall use the term 'object' for an element of a set and the term 'operation' for an element of a group.

Definition [a] 3.2.3.8. Let G be a group, A a set of objects $\mathbf{S}_i, \mathbf{S}_j, \mathbf{S}_k, \ldots$ and $\varphi : G \times \mathsf{A} \to \mathsf{A}$ a mapping that assigns to an ordered pair $(g, \mathbf{S}_i)$, where $g \in G$, S_i and S_i are objects of the set A:

$$\varphi : (g, \mathbf{S}_i) \mapsto \mathbf{S}_k, \quad g \in G, \quad \mathbf{S}_i, \mathbf{S}_k \in \mathsf{A}. \tag{3.2.3.46}$$

The ordered pair $(g, \mathbf{S}_i)$ can often be written simply as a product $g\mathbf{S}_i$ and the mapping as an equation. Then the relation (3.2.3.46) can be expressed in a simpler form:

$$g\mathbf{S}_i = \mathbf{S}_k, \quad g \in G, \ \mathbf{S}_i, \mathbf{S}_k \in \mathsf{A}. \tag{3.2.3.47}$$

If the mapping (3.2.3.46), expressed in this condensed way, fulfils two additional conditions,

$$e\mathbf{S}_i = \mathbf{S}_i \text{ for any } \mathbf{S}_i \in \mathsf{A}, \tag{3.2.3.48}$$

where e is the identity operation (unit element) of G, and

$$h(g\mathbf{S}_i) = (hg)\mathbf{S}_i \text{ for any } h, g \in G \text{ and any } \mathbf{S}_i \in \mathsf{A}, \tag{3.2.3.49}$$

then the mapping φ is called an *action* (or *operation*) *of a group G on a set* A, or just a *group action*.

We must note that the replacement of the explicit mapping (3.2.3.46) by a contracted version (3.2.3.47) is not always possible (see Example [aS] 3.2.3.11).

The condition (3.2.3.49) requires that the first action $g\mathbf{S}_i = \mathbf{S}_k$ followed by the second action $h\mathbf{S}_k = \mathbf{S}_m$ gives the same result as if one first calculates the product $hg = p$ and then applies it to $\mathbf{S}_i$, $p\mathbf{S}_i = \mathbf{S}_m$.

When a group G, a set A, and a mapping φ fulfil the requirements (3.2.3.47) to (3.2.3.49), one says that G *acts* or *operates on* A and the set A is called a *G-set*.

Example [aC] 3.2.3.9. We shall examine the action of an isometry g on an ideal infinite crystal in the three-dimensional space. Let us choose four points (atoms) of the crystal that define three non-coplanar vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ (*e.g.* basic lattice translations). These vectors will specify the *orientation of the crystal in space*. Let g be a point-group operation. This isometry g transforms (moves) points of the crystal to new positions and changes the orientation of the crystal to a new orientation specified by vectors $\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3$,

$$\mathbf{a}'_i = \sum_{j=3}^{3} D(g)_{ji}\mathbf{a}_j, \quad i = 1, 2, 3, \tag{3.2.3.50}$$

where $D(g)_{ji}$ are coefficients of a 3×3 matrix representing the operation g. For non-trivial operations g, the resulting vectors $\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3$ always differ from the initial ones. If g is an improper rotation (rotoinversion), then these vectors have an opposite handedness to the vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of the initial orientation and, for enantiomorphous crystals, the transformed crystal is an enantiomorphous form of the crystal in the initial orientation.

We choose a *reference coordinate system* defined by the origin O and by three non-coplanar basis vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$. By the *state* $\boldsymbol{S}$ *of a crystal* we shall understand, in a continuum description, the set of all its properties expressed by components of physical property (matter) tensors in the reference coordinate system or, in a microscopic description, the positions of atoms in the elementary unit cell expressed in the reference coordinate system. States defined in this way may change with temperature and external fields, and also with the orientation of the crystal in